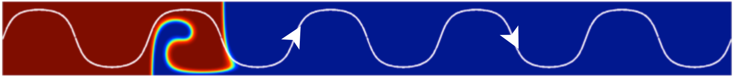
Reactive front propagation in periodic flows for fast reaction and small diffusivity

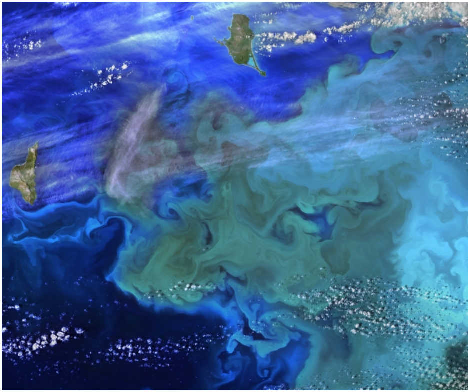
Alexandra Tzella
University of Birmingham



with Jacques Vanneste, University of Edinburgh

Reactive tracers in environmental flows

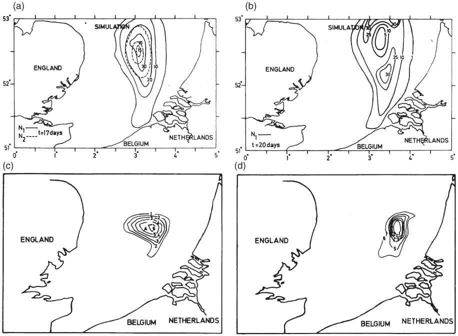
- Reactive tracers can propagate much more rapidly than a passive tracer in the same environment.
- Often in the form of localized, strongly inhomogeneous structures associated with reactive fronts.



Phytoplankton bloom off the coast of Alaska (NASA's Goddard Space, Sept. 22, 2014).

Reactive fronts in environmental flows

- Classic example of reactive front: the Fisher-Kolmogorov travelling-wave.
- Employed to explain observations of the spread of a phytoplankton in the North Sea for a weak surface flow.



Wyatt (1973), Martin (2003)

Reactive fronts in the absence of a flow

Reaction-diffusion with Fisher-Kolmogorov nonlinearity

$$\partial_t \theta(\boldsymbol{x}, t) = \kappa \Delta \theta(\boldsymbol{x}, t) + \frac{1}{\tau} \theta(1-\theta), \quad \theta(\boldsymbol{x}, 0) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases}$$

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$\theta(\boldsymbol{x}, t) = 0$ is an unstable solution (growth)

$\theta(\boldsymbol{x}, t) = 1$ is a stable solution (saturation)

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At large times, a front is established:

$$\theta(x, t) \to \Theta(x - c_0 t), \quad \text{when } t \gg 1.$$

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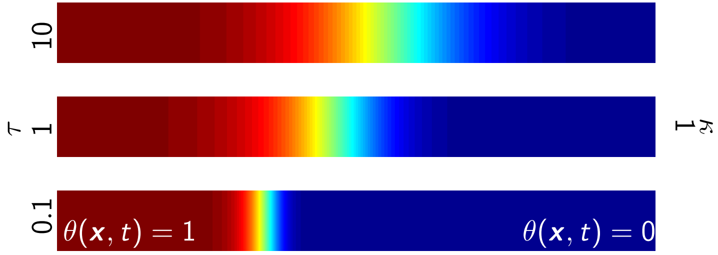

Reactive fronts in shear and cellular flows

Reaction-diffusion-advection with Fisher-Kolmogorov nonlinearity

$$\partial_t \theta(\boldsymbol{x}, t) + \boldsymbol{u}(\boldsymbol{x}) \cdot \nabla \theta(\boldsymbol{x}, t) = \mathrm{Pe}^{-1} \Delta \theta(\boldsymbol{x}, t) + \mathrm{Da}\, \theta(1 - \theta)$$

where

$$\mathrm{Pe} = V\ell/\kappa \quad \text{and} \quad \mathrm{Da} = \ell/V\tau$$

and $\boldsymbol{u} = (u(y), 0)$ or

$$\boldsymbol{u} = \nabla^{\perp}\psi \quad \text{with} \quad \psi = -Uy - \sin(x)\sin(y)$$

in a channel geometry (analysis for unbounded 2D domain is similar)

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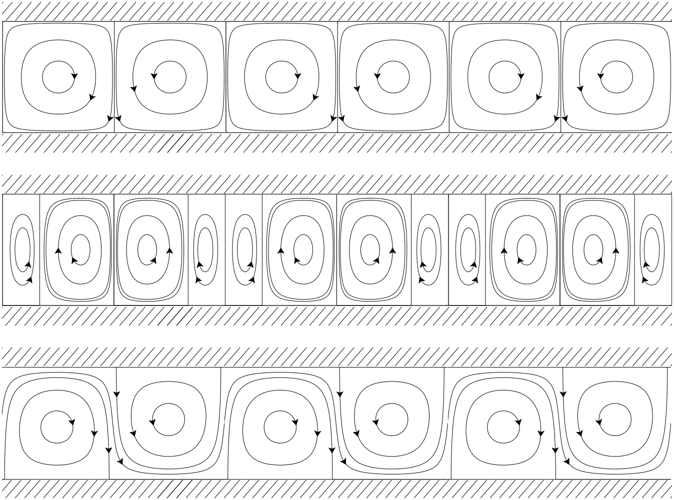

Reactive fronts in shear and cellular flows

At large times, a pulsating front is established:

$$\theta(x, y, t) \to \Theta(x - ct, x, y), \quad \text{when } t \gg 1.$$

where Θ is 2π-periodic in the second variable. Berestycki & Hamel (2002)

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Examples obtained for varying Da, $\mathrm{Pe} = 250$ and $U = 0$

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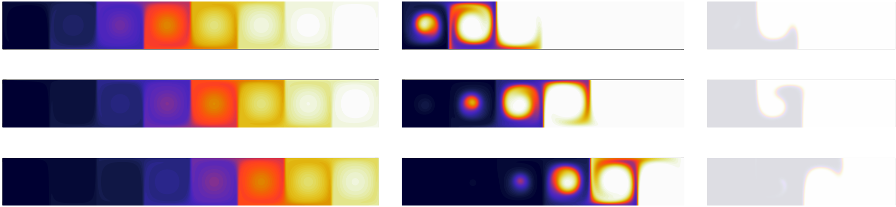

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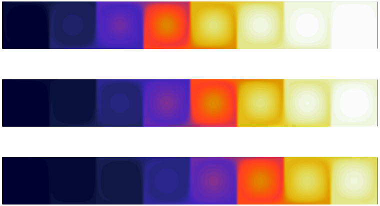
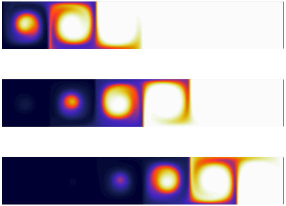


$\mathrm{Da} = 4 \times 10^{-2}$



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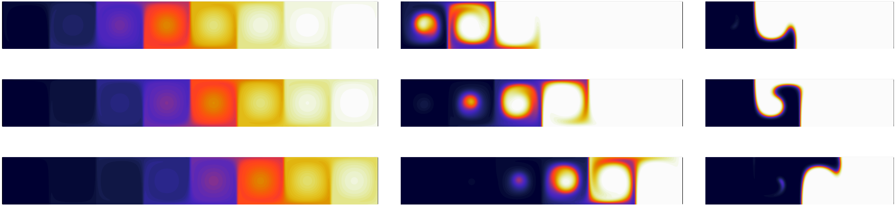

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What is the front speed c as a function of Pe and Da?
(when $\mathrm{Pe} \gg 1$)

Multiscale methods

Focus on advection-diffusion only:

$$\partial_t \theta(\boldsymbol{x}, t) + \boldsymbol{u}(\boldsymbol{x}) \cdot \nabla \theta(\boldsymbol{x}, t) = \mathrm{Pe}^{-1} \Delta \theta(\boldsymbol{x}, t).$$

For $t \gg 1$, the bulk behaviour is diffusive:

$$\partial_t \theta(x, t) + U \partial_x \theta = \kappa_{\text{eff}}\, \partial_x^2 \theta(x, t),$$

where the effective diffusivity κ_{eff} depends on $\boldsymbol{u}$.

For sudden localised release, predicts Gaussian concentration:

$$\theta(x, t) \sim e^{-(x-Ut)^2/(4\kappa_{\text{eff}} t)}.$$

- Accurate for $|x - Ut| = O(t^{1/2})$.
- Fails in the tails, $|x - Ut| \gg O(t^{1/2})$.
- Can capture the tails $|x - Ut| = O(t)$ using large deviations:

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(see Haynes & Vanneste (2014i,ii))

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The eigenvalue problem for the speed

Put back reactions: Linearising around the tip of the front, $\theta \approx 0$

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For $t \gg 1$ we employ the large-deviation form for the passive tracer:

$$\theta(\boldsymbol{x}, t) \approx e^{-t(g(c) - \mathrm{Da})} \phi(x, y) \quad \text{where } c = \frac{x}{t} = O(1)$$
$$= \begin{cases} \infty, & \text{for } c < g^{-1}(\mathrm{Da}) \\ 0, & \text{for } c > g^{-1}(\mathrm{Da}) \end{cases}$$

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We solve for $g(c)$ via an eigenvalue equation

$$f(q)\phi = \mathrm{Pe}^{-1}\Delta\phi - (u_1, u_2)\cdot\nabla\phi - 2\mathrm{Pe}^{-1}q\partial_x\phi + (u_1 q + \mathrm{Pe}^{-1}q^2)\phi,$$

where f is the Legendre transform of g

$$g(c) = \sup_{q>0}(qc - f(q)),$$

and $\phi(x, y)$ is 2π-periodic in x with $\partial_y\phi = 0$ at $y = 0, 1$.

For $\boldsymbol{u} = \mathbf{0}$, $f(q) = \mathrm{Pe}^{-1}q^2$ which recovers classic result

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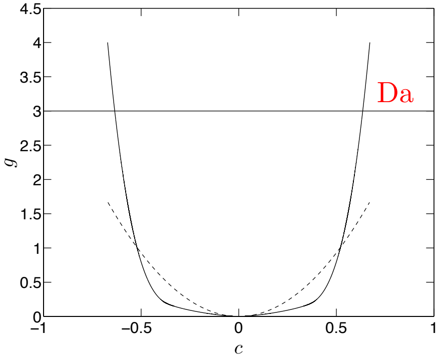
Example: $\mathrm{Pe} = 250$, $U = 0$



Near the origin, effective diffusivity approximation applies:

$$g(c) \approx \frac{\sqrt{\mathrm{Pe}}}{4} c^2$$

Childress (1979), Shraiman (1987), Soward (1987)

Away from the origin, reduced models using matched asymptotics

Haynes & Vanneste (2014), Tzella & Vanneste (2015)

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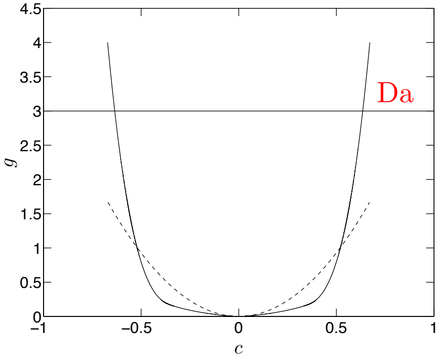

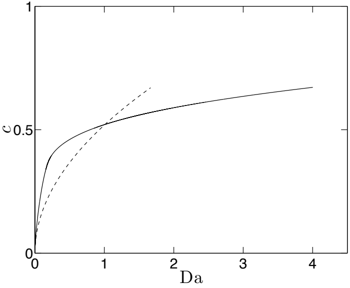

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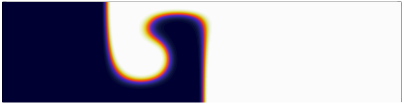
$\mathrm{Da} = \mathsf{O}(\mathrm{Pe})$, $c = \mathscr{C}(\mathrm{Da}/\mathrm{Pe})$



In the limit of small molecular diffusivity and fast reaction i.e., when

$$\mathrm{Pe},\ \mathrm{Da} \gg 1, \quad \mathrm{Da}/\mathrm{Pe} = c_0^2/4 = O(1),$$

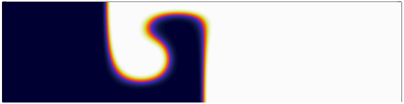
the solution to

$$\partial_t \theta + \boldsymbol{u} \cdot \nabla \theta = \mathrm{Pe}^{-1}\, \Delta \theta + \mathrm{Da}\, \theta.$$

can be approximated using a WKB approximation:

$$\theta(\boldsymbol{x}, t) \sim \mathrm{e}^{-\mathrm{Pe}\, \mathscr{I}(\boldsymbol{x}, t, c_0)}$$
$$\sim \mathrm{e}^{-\mathrm{Pe}\, t\, (\mathscr{G}(c) - c_0^2)/4} \quad \text{for } t \gg 1.$$

$\mathrm{Da} = O(\mathrm{Pe})$, $c = \mathscr{C}(\mathrm{Da}/\mathrm{Pe})$



At leading order, we obtain

$$\partial_t \mathscr{I} + \mathscr{H}(\nabla \mathscr{I}, \boldsymbol{x}, c_0) = 0 \quad \text{with } \mathscr{H}(\boldsymbol{p}, \boldsymbol{x}, c_0) = |\boldsymbol{p}|^2 + \boldsymbol{u}(\boldsymbol{x}) \cdot \boldsymbol{p} + c_0^2/4$$

where $\mathscr{I}(x, y, 0) = 0$ for $x \leq 0$ and ∞ otherwise.

The front interface is given by

$$\mathscr{I}(\boldsymbol{x}, t, c_0) = 0.$$

Variational formulation for the speed

The solution to the Hamilton–Jacobi equation is given by

$$\mathscr{I}(\boldsymbol{x}, T, c_0) = \frac{1}{4}\left(\inf_{\boldsymbol{X}(\cdot)} \int_0^T |\dot{\boldsymbol{X}}(t) - \boldsymbol{u}(\boldsymbol{X}(t))|^2 \,\mathrm{d}t - c_0^2 T\right),$$

$$\text{subject to } \boldsymbol{X}(0) = (0, \cdot), \quad \boldsymbol{X}(T) = \boldsymbol{x}.$$

For $T \gg 1$, the front propagates at the constant speed c obtained from

$$\mathscr{G}(c) = \lim_{T\to\infty} \frac{1}{T} \inf_{\boldsymbol{X}(\cdot)} \int_0^T |\dot{\boldsymbol{X}}(t) - \boldsymbol{u}(\boldsymbol{X}(t))|^2 \,\mathrm{d}t$$

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where the dependence on the specific value of y is dropped.

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Variational formulation for the speed

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$$\mathscr{G}(c) = \frac{1}{\tau} \inf_{\boldsymbol{X}(\cdot)} \int_0^\tau |\dot{\boldsymbol{X}}(t) - \boldsymbol{u}(\boldsymbol{X}(t))|^2 \, \mathrm{d}t,$$

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and use $\mathscr{G}(c) = c_0^2$.

Alternatively,

$$c = \frac{2\pi}{\tau}, \quad \text{where} \quad \tau = \inf_{\boldsymbol{X}(\cdot)} \tau \quad \text{with} \quad \boldsymbol{X}(\tau) = \boldsymbol{X}(0) + (2\pi, 0)$$

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Cellular flow ($U = 0$): Trajectories

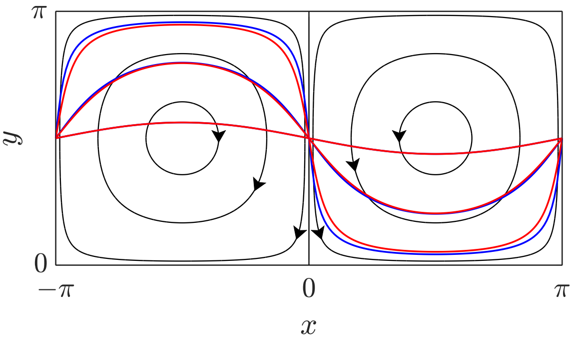


Figure: Minimising periodic trajectories calculated numerically for $c_0 = 0.1$, $c_0 = 1$ and $c_0 = 10$. They become closer to the straight line $y = \pi/2$ as c_0 increases.

Cellular flow ($U = 0$): Speed

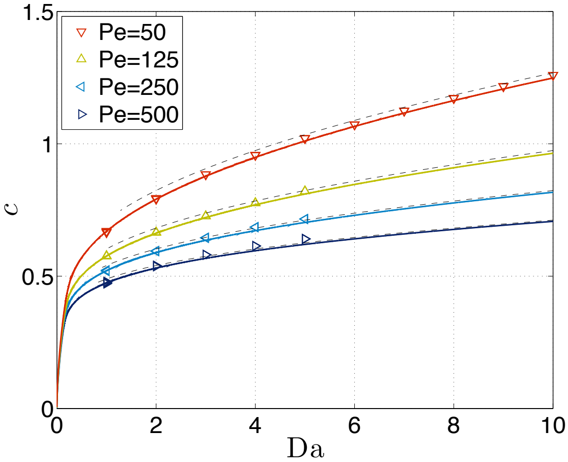
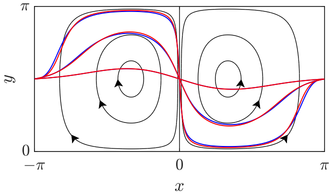
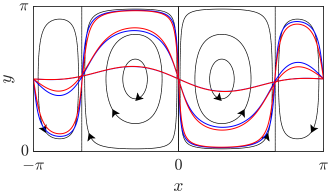


Figure: Comparison between asymptotic and numerical results of the front speed c when $\mathrm{Da} = O(\mathrm{Pe})$ for various values of $\mathrm{Pe} \gg 1$.

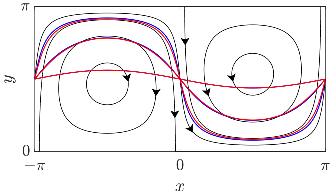
Cellular flow ($U \neq 0$): Trajectories



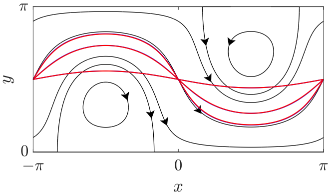
(a) $A = 0.5,\ U = 0$



(b) $A = 1,\ U = 0$



(c) $A = 0,\ U = 0.1$



(d) $A = 0,\ U = 0.5$

Figure: Effect of small-scale perturbations and a mean flow.

Conclusions

- Large deviation theory is a neat way to obtain the front speed in periodic flows:
  Letting $\theta \asymp \exp[-t(g(x/t) - \mathrm{Da})]$ gives:

  $$c = g^{-1}(\mathrm{Da}),$$

  where the rate function g is calculated by solving an eigenvalue problem.
- When the reactions are (very) weak, effective diffusivity may be used to approximate the front speed.
- When the reactions are strong, the front speed may be expressed in terms of periodic trajectories that minimise the time of travel across a period of the flow.

Outlook

- Geophysical flows.
- Other plankton ecosystems.

Thank you for your attention!

Tzella & Vanneste (2014) Phys. Rev. E 90, 011001(R);

Tzella & Vanneste (2015) SIAM J. Appl. Math, 75(4), 1789-1816;

Tzella & Vanneste (2018) in prep.

Cellular flow ($U \neq 0$): Speed

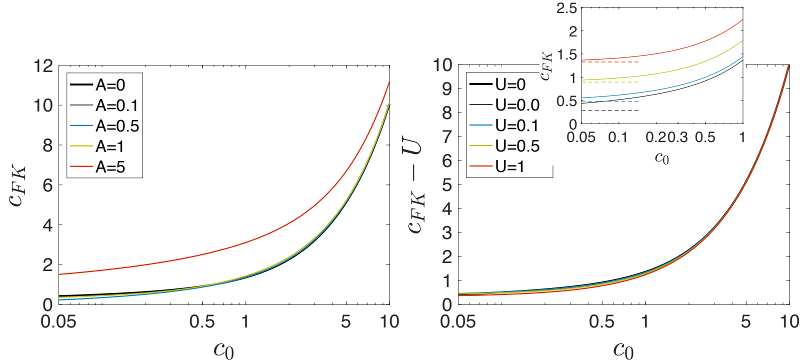


Figure: The difference between c and U, as a function of the bare speed c_0 for (left) various values of A with $U = 0$ and (right) various values of U with $A = 0$.